

09965766

d his

(FILE 'HOME' ENTERED AT 17:27:25 ON 10 JUL 2002)

FILE 'REGISTRY' ENTERED AT 17:27:32 ON 10 JUL 2002

L1 STRUCTURE UPLOADED
L2 15 S L1
L3 STRUCTURE UPLOADED
L4 15 S L3
L5 326 S L3 SSS FULL

FILE 'STNGUIDE' ENTERED AT 17:33:52 ON 10 JUL 2002

FILE 'REGISTRY' ENTERED AT 17:35:37 ON 10 JUL 2002

L6 STRUCTURE UPLOADED
L7 7 S L6 SUB=L5 SAMPLE
L8 208 S L6 SSS FULL SUB=L5

FILE 'CAPLUS' ENTERED AT 17:37:54 ON 10 JUL 2002

L9 117 S L8

FILE 'STNGUIDE' ENTERED AT 17:38:43 ON 10 JUL 2002

FILE 'REGISTRY' ENTERED AT 17:39:34 ON 10 JUL 2002

L10 STRUCTURE UPLOADED
L11 5 S L10 SUB=L5 SAMPLE

FILE 'STNGUIDE' ENTERED AT 17:41:24 ON 10 JUL 2002

FILE 'REGISTRY' ENTERED AT 17:42:59 ON 10 JUL 2002

L12 STRUCTURE UPLOADED
L13 5 S L12 SUB=L5 SAMPLE

FILE 'STNGUIDE' ENTERED AT 17:44:44 ON 10 JUL 2002

FILE 'REGISTRY' ENTERED AT 17:46:34 ON 10 JUL 2002

L14 STRUCTURE UPLOADED
L15 1 S L14 SUB=L5 SAMPLE
L16 50 S L14 SUB=L5 FULL

FILE 'CAPLUS' ENTERED AT 17:48:07 ON 10 JUL 2002

L17 4 S L16

FILE 'CAOLD' ENTERED AT 17:49:24 ON 10 JUL 2002

L18 1 S L16
L19 41 S L5 NOT L8

FILE 'CAPLUS' ENTERED AT 17:51:57 ON 10 JUL 2002

L20 204 S L5
L21 87 S L20 NOT L8
L22 87 S L20 NOT L9

FILE 'STNGUIDE' ENTERED AT 17:53:12 ON 10 JUL 2002

L23 0 S MEISSNER H/IN

FILE 'CAPLUS' ENTERED AT 17:56:02 ON 10 JUL 2002

L24 0 S MEISSNER H/IN
E MEISSNER HELMUT/IN
L25 4 S E3
L26 87 S L21 NOT L25
L27 87 S L22 NOT L25

FILE 'STNGUIDE' ENTERED AT 17:59:41 ON 10 JUL 2002

FILE 'REGISTRY' ENTERED AT 18:01:47 ON 10 JUL 2002

L28 STRUCTURE UPLOADED
L29 5 S L28 SUB=L5 SAMPLE
L30 162 S L28 SUB=L5 FULL

FILE 'CAPLUS' ENTERED AT 18:03:43 ON 10 JUL 2002

L31 55 S L30
L32 79 S L22 NOT L31
L33 0 S L32 NOT L20

FILE 'REGISTRY' ENTERED AT 18:06:13 ON 10 JUL 2002

L34 164 S L5 NOT L30
L35 136 S L34 NOT L16
L36 99 S L35 NOT HYDROXY

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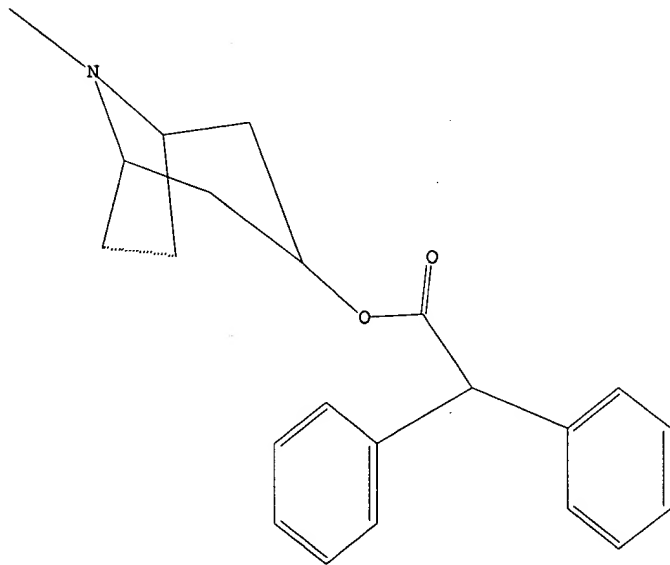
L37 85 S L36 NOT TELOIDINE
L38 84 S L37 NOT C29 H31 N O4 . CL H/MF
L39 81 S L38 NOT AMINO
L40 5 S L29 NOT DIETHYLAMINO
L41 81 S L39 NOT DIETHYLAMINO
L42 67 S L41 NOT BENZILI?
L43 66 S L42 NOT NAPHTH?
L44 63 S L43 NOT DIMETHOXY

FILE 'CAPLUS' ENTERED AT 18:16:47 ON 10 JUL 2002
L45 104 S L44
S L45 AND C22 H25 N O2 . CL H/MF

FILE 'REGISTRY' ENTERED AT 18:17:35 ON 10 JUL 2002
L46 156 S C22 H25 N O2 . CL H/MF

FILE 'CAPLUS' ENTERED AT 18:17:35 ON 10 JUL 2002
L47 184 S L46
L48 5 S L45 AND L47
L49 99 S L45 NOT L48
L50 1 S L49 AND FLUORO
L51 98 S L49 NOT L50
L52 3 S L51 AND PATENT/DT
L53 3 S L52 NOT L25
L54 95 S L51 NOT L53
L55 14 S L54 NOT 6878-98-4/RN
L56 204 S L5

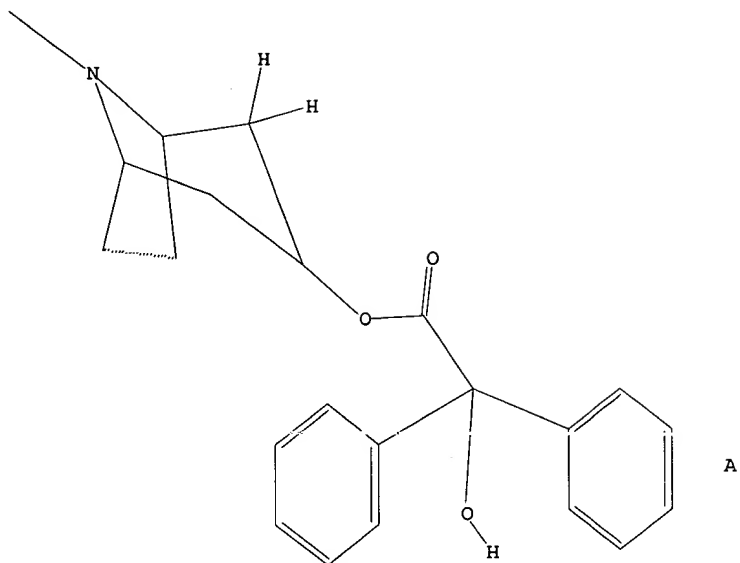
=> d 11
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

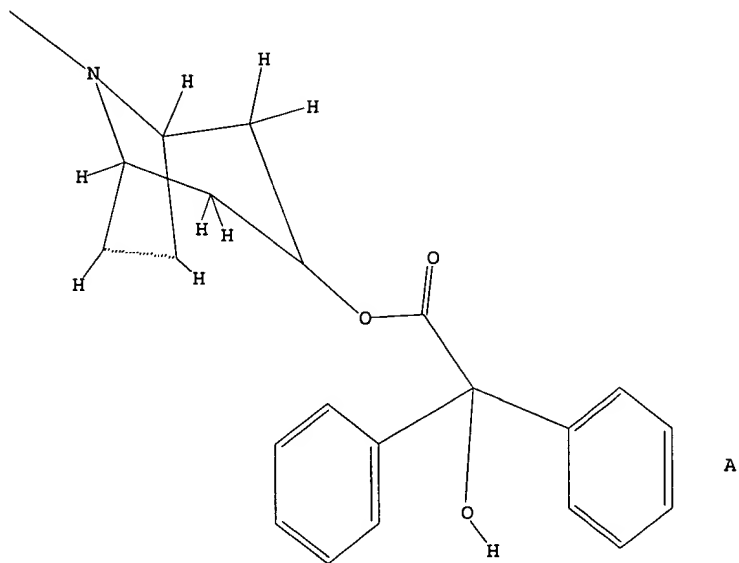
=> d 110
L10 HAS NO ANSWERS
L10 STR

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Structure attributes must be viewed using STN Express query preparation.

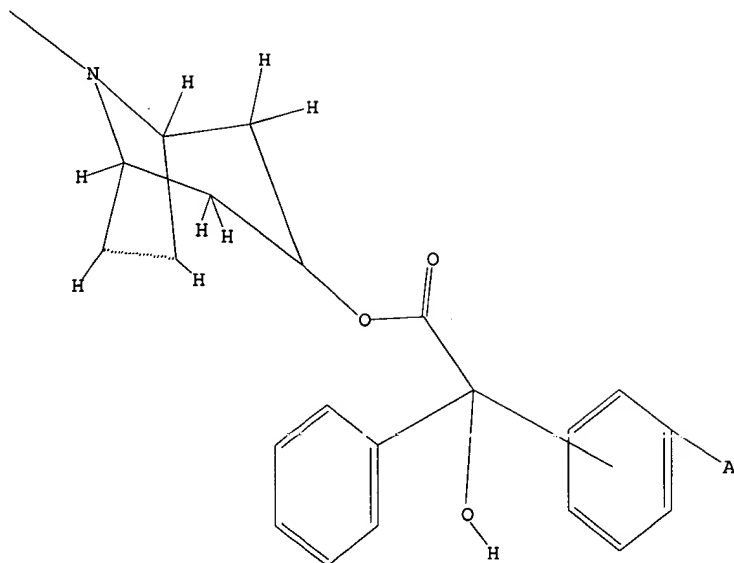
=> d l12
L12 HAS NO ANSWERS
L12 STR



Structure attributes must be viewed using STN Express query preparation.

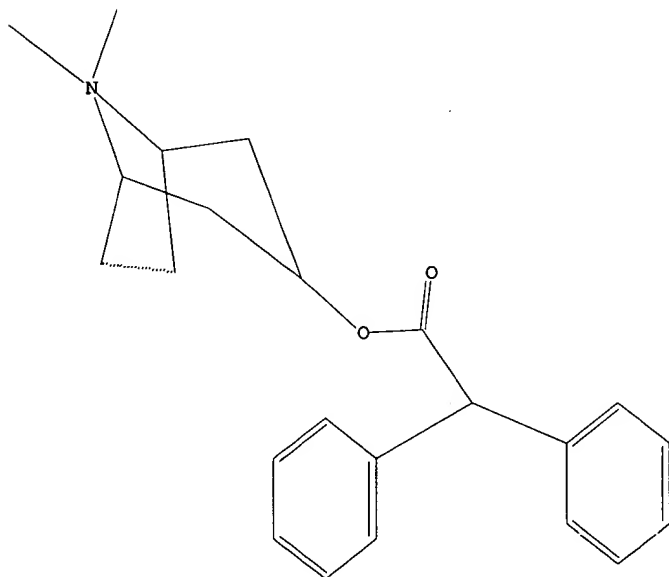
=> d l14
L14 HAS NO ANSWERS
L14 STR

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Structure attributes must be viewed using STN Express query preparation.

=> d 128
L28 HAS NO ANSWERS
L28 STR



+ 014

09965766

L17 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2002 ACS
AN 2002:291678 CAPLUS
DN 136:310064
TI Procedures for the production of new anticholinergics, and their use as
drugs
IN Meissner, Helmut; Morschhaeuser, Gerd; Pieper, Helmut; Pohl, Gerald;
Reichl, Richard; Speck, Georg
PA Boehringer Ingelheim Pharma K.-G., Germany
SO Ger. Offen., 28 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10050995	A1	20020418	DE 2000-10050995	20001014
	WO 2002032898	A2	20020425	WO 2001-EP11243	20010928
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PRAI	DE 2000-10050995	A	20001014		
OS	CASREACT 136:310064; MARPAT 136:310064				
GI					

this apr 11

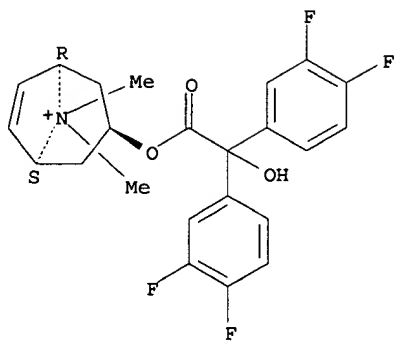
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention concerns new anticholinergics I [A = CH₂CH₂, CH:CH, oxirane-2,3-diyl; X- = simple anion; R₁, R₂ = C₁-4-alkyl, C₁-4-hydroxyalkyl, C₁-4-haloalkyl; R₃, R₄, R₅, R₆ = H, C₁-4-alkyl, C₁-4-alkoxy, OH, CF₃, CN, NO₂, halogen, whereby at least one of R₃ - R₆ .noteq. H] as an optically active isomers, as mixts. of enantiomers or as racemates, procedures for their prodn. as well as their use as drugs. Thus, the diphenylglycolate II.cntdot.Br- was prepd. from tropenol via transesterification of Et bis(3,4-difluorophenyl)glycolate followed by quaternization with MeBr in CH₂Cl₂/MeCN. Pharmaceutical formulations, for the use of I in tablets, ampuls, aerosols, solns. and inhalants, are presented.

IT 412030-72-9P 412030-73-0P 412030-74-1P
412030-75-2P 412030-76-3P 412030-77-4P
412030-78-5P 412030-79-6P 412030-80-9P
412030-81-0P 412030-82-1P 412030-83-2P
412030-84-3P 412030-85-4P 412030-86-5P
412030-87-6P 412030-88-7P 412030-89-8P
412032-24-7P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepd. of alkaloid diphenylglycolates as anticholinergics)
RN 412030-72-9 CAPLUS
CN 8-Azoniabicyclo[3.2.1]oct-6-ene, 3-[[bis(3,4-difluorophenyl)hydroxyacetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

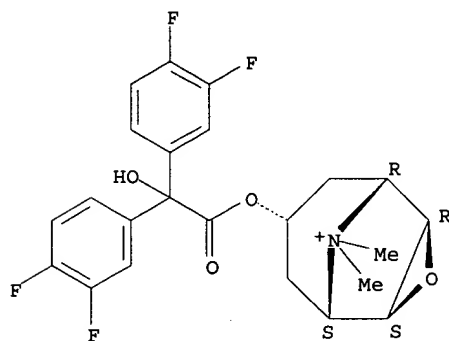
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● Br⁻

RN 412030-73-0 CAPLUS
CN 3-Oxa-9-azoniatricyclo[3.3.1.0^{2,4}]nonane, 7-[[bis(3,4-difluorophenyl)hydroxyacetyl]oxy]-9,9-dimethyl-, bromide, (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)- (9CI) (CA INDEX NAME)

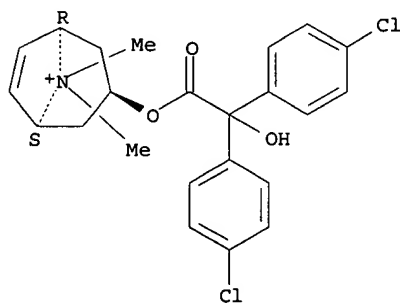
Relative stereochemistry.



● Br⁻

RN 412030-74-1 CAPLUS
CN 8-Azoniabicyclo[3.2.1]oct-6-ene, 3-[[bis(4-chlorophenyl)hydroxyacetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

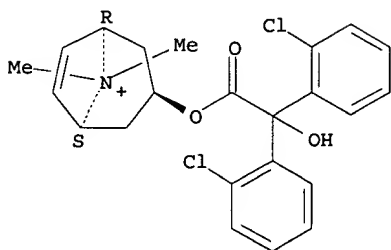


● Br⁻

RN 412030-75-2 CAPLUS
CN 8-Azoniabicyclo[3.2.1]oct-6-ene, 3-[[bis(2-chlorophenyl)hydroxyacetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

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Absolute stereochemistry.

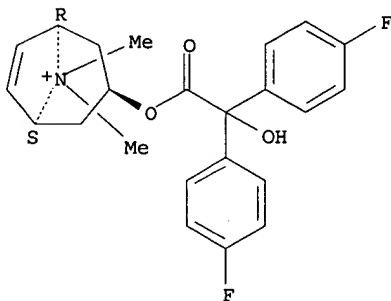


● Br⁻

RN 412030-76-3 CAPLUS

CN 8-Azoniabicyclo[3.2.1]oct-6-ene, 3-[[bis(4-fluorophenyl)hydroxyacetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

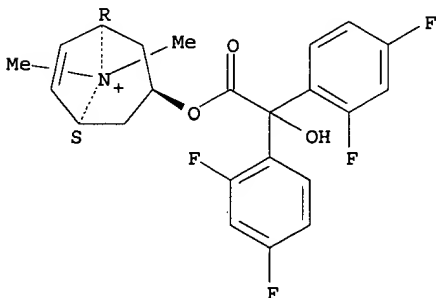


● Br⁻

RN 412030-77-4 CAPLUS

CN 8-Azoniabicyclo[3.2.1]oct-6-ene, 3-[[bis(2,4-difluorophenyl)hydroxyacetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



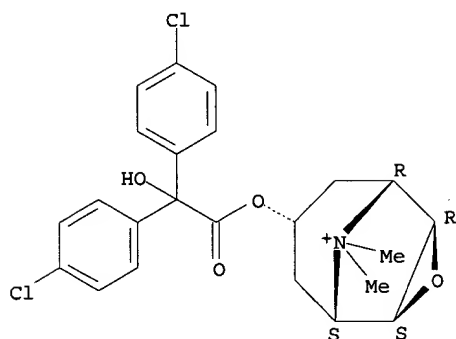
● Br⁻

RN 412030-78-5 CAPLUS

CN 3-Oxa-9-azoniatricyclo[3.3.1.0^{2,4}]nonane, 7-[[bis(4-chlorophenyl)hydroxyacetyl]oxy]-9,9-dimethyl-, bromide, (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)- (9CI) (CA INDEX NAME)

09965766

Relative stereochemistry.

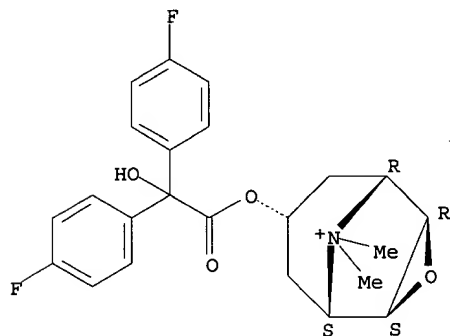


● Br⁻

RN 412030-79-6 CAPLUS

CN 3-Oxa-9-azoniatricyclo[3.3.1.0^{2,4}]nonane, 7-[[bis(4-fluorophenyl)hydroxyacetyl]oxy]-9,9-dimethyl-, bromide, (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

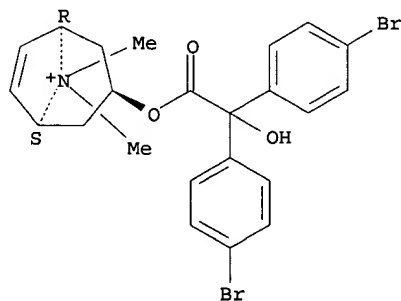


● Br⁻

RN 412030-80-9 CAPLUS

CN 8-Azoniabicyclo[3.2.1]oct-6-ene, 3-[[bis(4-bromophenyl)hydroxyacetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



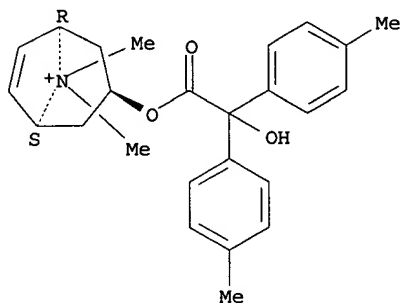
● Br⁻

RN 412030-81-0 CAPLUS

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CN 8-Azoniabicyclo[3.2.1]oct-6-ene, 3-[[hydroxybis(4-methylphenyl)acetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

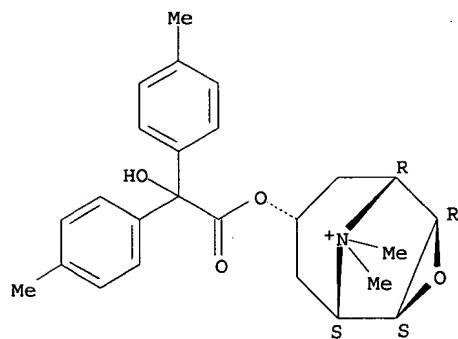


● Br⁻

RN 412030-82-1 CAPLUS

CN 3-Oxa-9-azoniatricyclo[3.3.1.0^{2,4}]nonane, 7-[[hydroxybis(4-methylphenyl)acetyl]oxy]-9,9-dimethyl-, bromide, (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

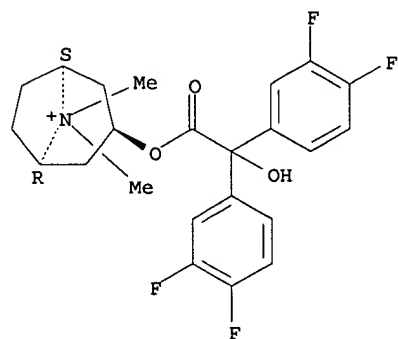


● Br⁻

RN 412030-83-2 CAPLUS

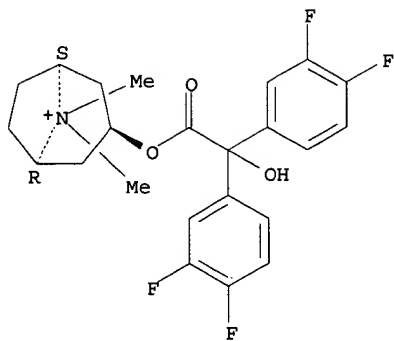
CN 8-Azoniabicyclo[3.2.1]octane, 3-[[bis(3,4-difluorophenyl)hydroxyacetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br⁻

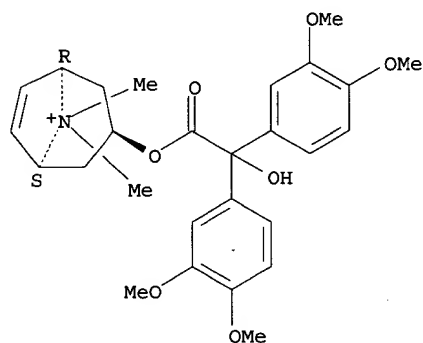
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● Br⁻

RN 412030-84-3 CAPLUS
CN 8-Azoniabicyclo[3.2.1]oct-6-ene, 3-[[bis(3,4-dimethoxyphenyl)hydroxyacetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

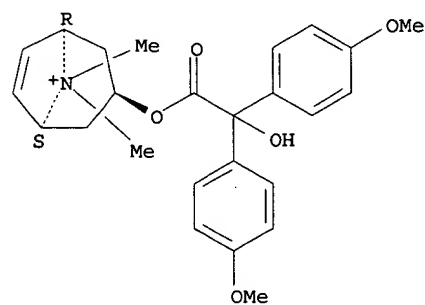
Absolute stereochemistry.



● Br⁻

RN 412030-85-4 CAPLUS
CN 8-Azoniabicyclo[3.2.1]oct-6-ene, 3-[[hydroxybis(4-methoxyphenyl)acetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

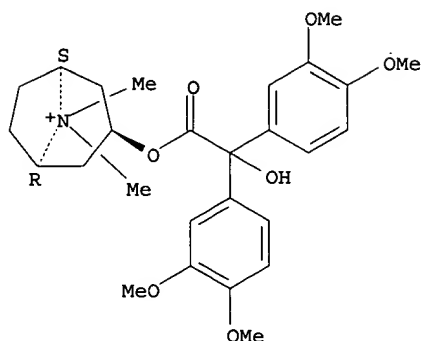


● Br⁻

RN 412030-86-5 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[[bis(3,4-dimethoxyphenyl)hydroxyacetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

09965766

Absolute stereochemistry.

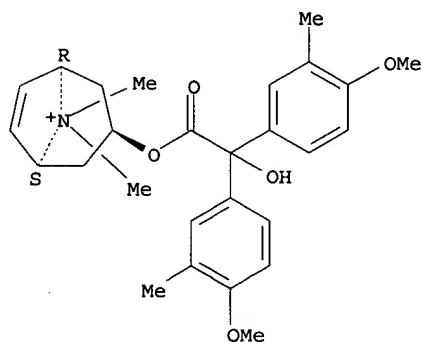


● Br⁻

RN 412030-87-6 CAPLUS

CN 8-Azoniabicyclo[3.2.1]oct-6-ene, 3-[[hydroxybis(4-methoxy-3-methylphenyl)acetyl]oxy]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

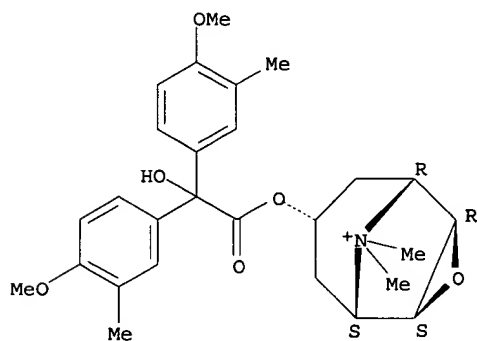


● Br⁻

RN 412030-88-7 CAPLUS

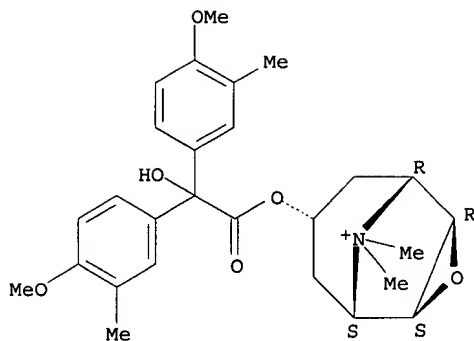
CN 3-Oxa-9-azoniatricyclo[3.3.1.02,4]nonane, 7-[[hydroxybis(4-methoxy-3-methylphenyl)acetyl]oxy]-9,9-dimethyl-, bromide, (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● Br⁻

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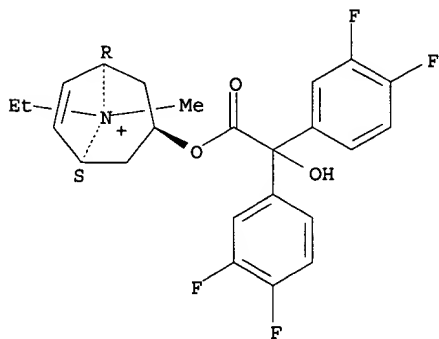


● Br⁻

RN 412030-89-8 CAPLUS

CN 8-Azoniabicyclo[3.2.1]oct-6-ene, 3-[[bis(3,4-difluorophenyl)hydroxyacetyl]oxy]-8-ethyl-8-methyl-, bromide, (3-endo,8-anti)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

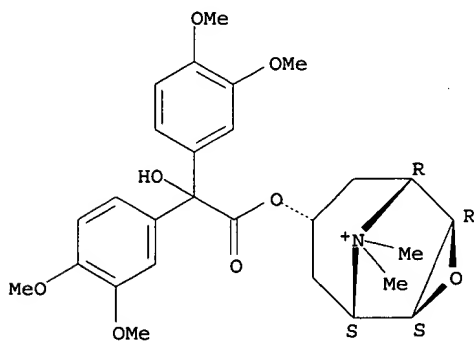


● Br⁻

RN 412032-24-7 CAPLUS

CN 3-Oxa-9-azoniatricyclo[3.3.1.0^{2,4}]nonane, 7-[[bis(3,4-dimethoxyphenyl)hydroxyacetyl]oxy]-9,9-dimethyl-, bromide, (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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IT 428868-87-5 428876-65-7 412030-93-4P
412030-94-5P 412030-95-6P 412030-96-7P

09965766

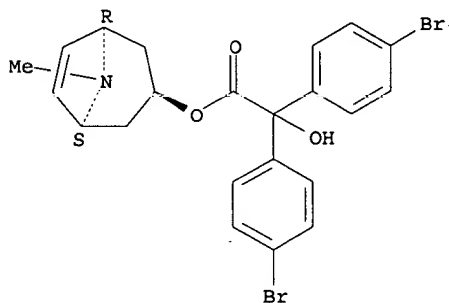
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412031-00-6P 412031-01-7P 412031-02-8P
412031-04-0P 412031-06-2P 412031-08-4P
412031-10-8P 412031-12-0P 412031-14-2P
412031-16-4P 412031-18-6P

RL: RCT (Reactant); SPN (Synthetic preparation)
(prepn. and quaternization with Me bromide; prepd. of alkaloid
diphenylglycolates as anticholinergics)

RN 428868-87-5 CAPLUS

CN Benzeneacetic acid, 4-bromo-.alpha.-(4-bromophenyl)-.alpha.-hydroxy-,
(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester (9CI) (CA INDEX
NAME)

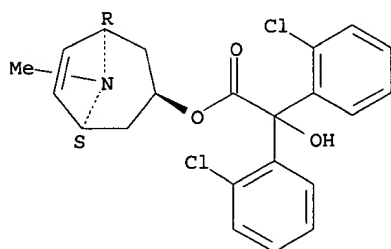
Absolute stereochemistry.



RN 428876-65-7 CAPLUS

CN Benzeneacetic acid, 2-chloro-.alpha.-(2-chlorophenyl)-.alpha.-hydroxy-,
(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester (9CI) (CA INDEX
NAME)

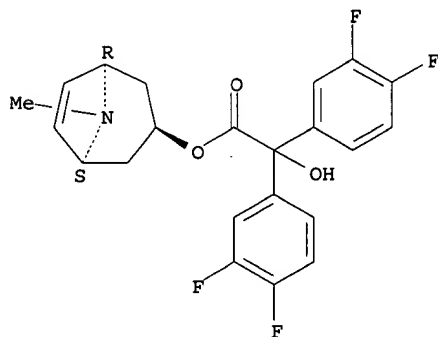
Absolute stereochemistry.



RN 412030-93-4 CAPLUS

CN Benzeneacetic acid, .alpha.-(3,4-difluorophenyl)-3,4-difluoro-.alpha.-
hydroxy-, (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

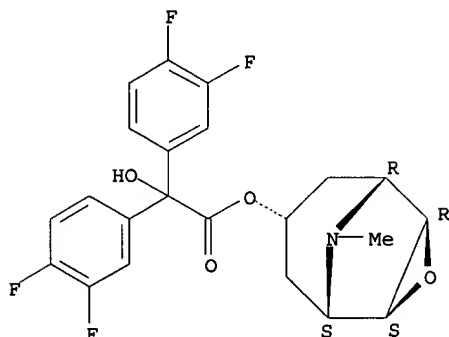


RN 412030-94-5 CAPLUS

CN Benzeneacetic acid, .alpha.-(3,4-difluorophenyl)-3,4-difluoro-.alpha.-
hydroxy-, (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)-9-methyl-3-oxa-9-
azatricyclo[3.3.1.0^{2,4}]non-7-yl ester (9CI) (CA INDEX NAME)

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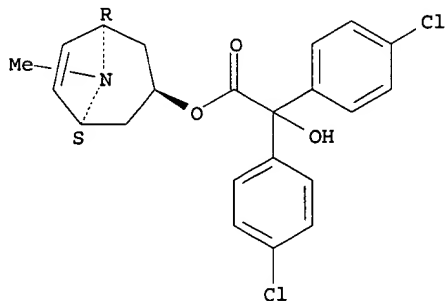
Relative stereochemistry.



RN 412030-95-6 CAPLUS

CN Benzeneacetic acid, 4-chloro-.alpha.-(4-chlorophenyl)-.alpha.-hydroxy-,
(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester (9CI) (CA INDEX
NAME)

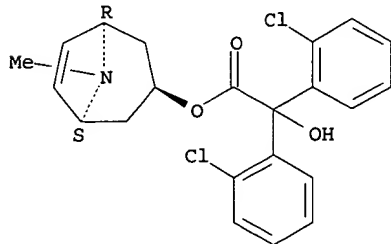
Absolute stereochemistry.



RN 412030-96-7 CAPLUS

CN Benzeneacetic acid, 2-chloro-.alpha.-(2-chlorophenyl)-.alpha.-hydroxy-,
(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester, hydrochloride
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



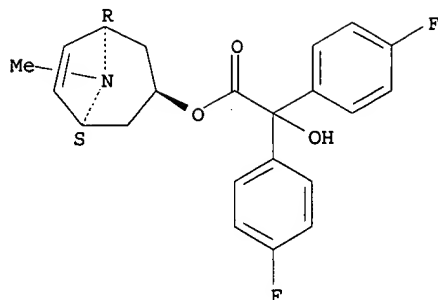
● HCl

RN 412030-97-8 CAPLUS

CN Benzeneacetic acid, 4-fluoro-.alpha.-(4-fluorophenyl)-.alpha.-hydroxy-,
(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester (9CI) (CA INDEX
NAME)

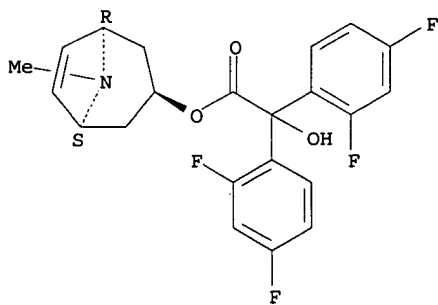
Absolute stereochemistry.

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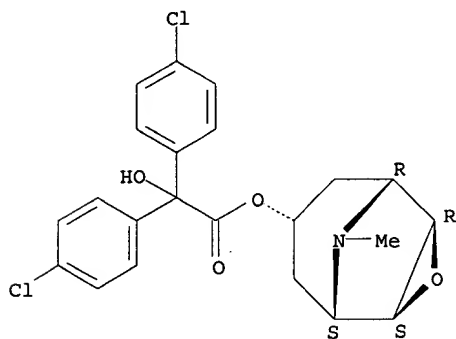
RN 412030-98-9 CAPLUS
CN Benzeneacetic acid, .alpha.-(2,4-difluorophenyl)-2,4-difluoro-.alpha.-hydroxy-, (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 412030-99-0 CAPLUS
CN Benzeneacetic acid, 4-chloro-.alpha.-(4-chlorophenyl)-.alpha.-hydroxy-, (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)-9-methyl-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]non-7-yl ester, hydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

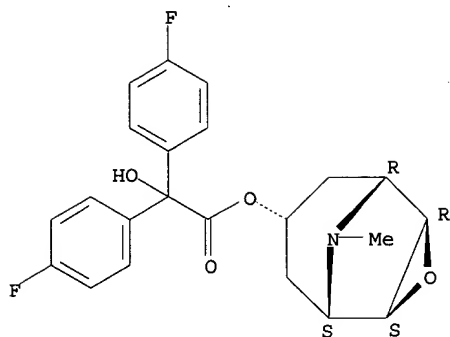


● HCl

RN 412031-00-6 CAPLUS
CN Benzeneacetic acid, 4-fluoro-.alpha.-(4-fluorophenyl)-.alpha.-hydroxy-, (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)-9-methyl-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]non-7-yl ester, hydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

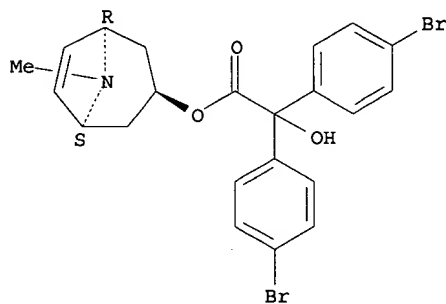
09965766



● HCl

RN 412031-01-7 CAPLUS
 CN Benzeneacetic acid, 4-bromo-.alpha.-(4-bromophenyl)-.alpha.-hydroxy-,
 (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester, hydrochloride
 (9CI) (CA INDEX NAME)

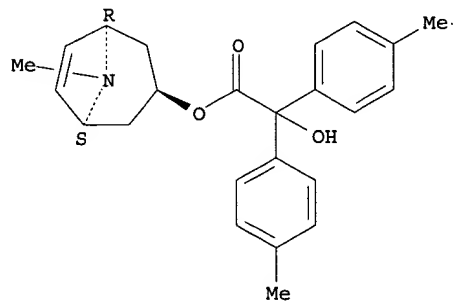
Absolute stereochemistry.



● HCl

RN 412031-02-8 CAPLUS
 CN Benzeneacetic acid, .alpha.-hydroxy-4-methyl-.alpha.-(4-methylphenyl)-,
 (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester, hydrochloride
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

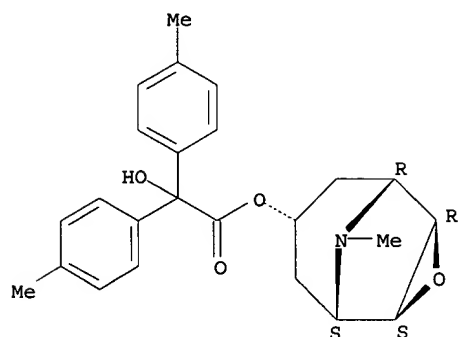


HCl

RN 412031-04-0 CAPLUS
 CN Benzeneacetic acid, .alpha.-hydroxy-4-methyl-.alpha.-(4-methylphenyl)-,
 (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)-9-methyl-3-oxa-9-
 azatricyclo[3.3.1.0^{2,4}]non-7-yl ester, hydrochloride (9CI) (CA INDEX
 NAME)

09965766

Relative stereochemistry.

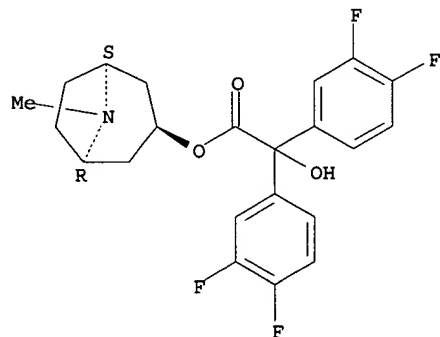


● HCl

RN 412031-06-2 CAPLUS

CN Benzeneacetic acid, .alpha.-(3,4-difluorophenyl)-3,4-difluoro-.alpha.-hydroxy-, (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester (9CI) (CA INDEX NAME)

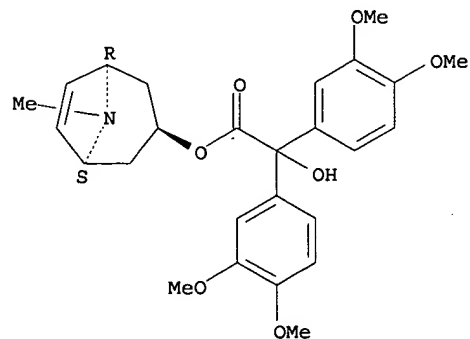
Absolute stereochemistry.



RN 412031-08-4 CAPLUS

CN Benzeneacetic acid, .alpha.-(3,4-dimethoxyphenyl)-.alpha.-hydroxy-3,4-dimethoxy-, (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

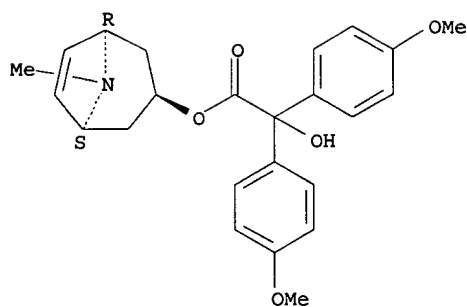


RN 412031-10-8 CAPLUS

CN Benzeneacetic acid, .alpha.-hydroxy-4-methoxy-.alpha.-(4-methoxyphenyl)-, (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester (9CI) (CA INDEX NAME)

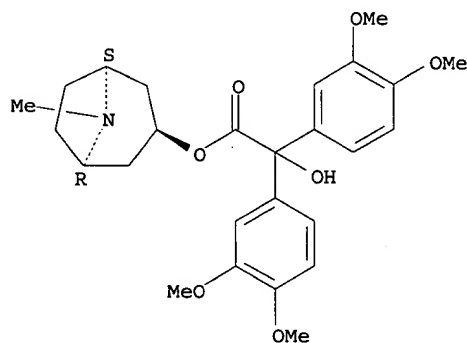
Absolute stereochemistry.

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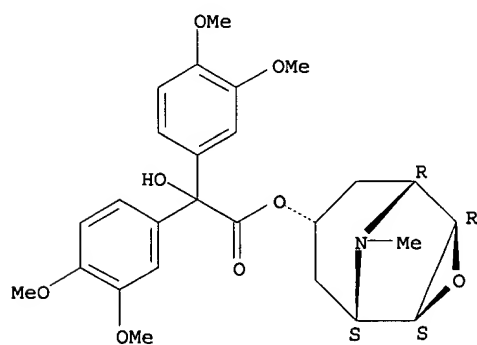
RN 412031-12-0 CAPLUS
CN Benzeneacetic acid, .alpha.-(3,4-dimethoxyphenyl)-.alpha.-hydroxy-3,4-dimethoxy-, (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 412031-14-2 CAPLUS
CN Benzeneacetic acid, .alpha.-(3,4-dimethoxyphenyl)-.alpha.-hydroxy-3,4-dimethoxy-, (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)-9-methyl-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]non-7-yl ester (9CI) (CA INDEX NAME)

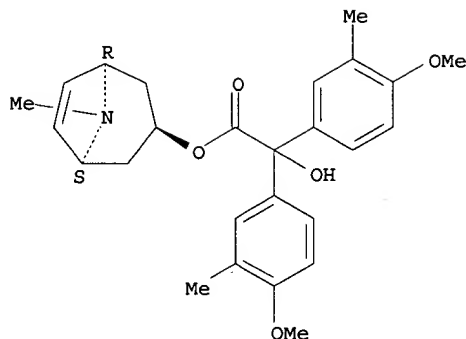
Relative stereochemistry.



RN 412031-16-4 CAPLUS
CN Benzeneacetic acid, .alpha.-hydroxy-4-methoxy-.alpha.-(4-methoxy-3-methylphenyl)-3-methyl-, (3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-6-en-3-yl ester (9CI) (CA INDEX NAME)

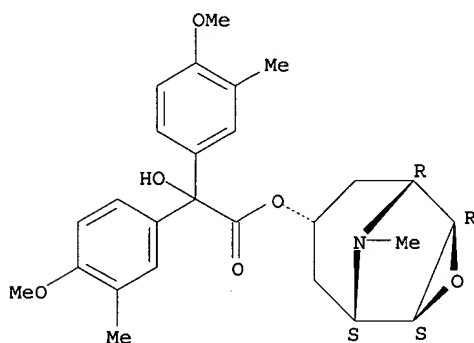
Absolute stereochemistry.

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RN 412031-18-6 CAPLUS
CN Benzeneacetic acid, .alpha.-hydroxy-4-methoxy-.alpha.-(4-methoxy-3-methylphenyl)-3-methyl-, (1.alpha.,2.beta.,4.beta.,5.alpha.,7.beta.)-9-methyl-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]non-7-yl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

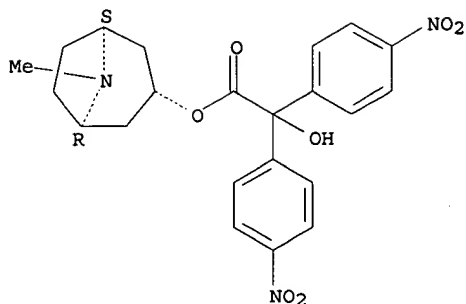


RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2002 ACS
AN 1995:971791 CAPLUS
DN 124:111207
TI Fluorinated tropanyl esters for application with PET
AU Emran, Ali M.; Lim, Jean-Luc; Flynn, Donna D.; Emran, Mohammad A.; Cherif, Abdallah; Yang, David
CS Health Science Center, University Texas, Houston, TX, 77030, USA
SO Chem. Views Imaging Cent., [Proc. Am. Chem. Soc. Symp.] (1995), Meeting Date 1993, 485-96. Editor(s): Emran, Ali M. Publisher: Plenum, New York, N. Y.
CODEN: 61ZBA7
DT Conference
LA English
AB The present study is aimed at the synthesis of muscarinic acetylcholine receptor ligands labeled with 18F. An in vitro evaluation of the biol. activity of the newly prepd. derivs. are included and the development of the appropriate synthetic methods detailed for labeling with 18F.
IT 172883-93-1 172883-94-2 172883-95-3
172883-98-6 172883-99-7 172884-00-3
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fluorinated tropanyl esters for application with PET)
RN 172883-93-1 CAPLUS
CN Benzeneacetic acid, .alpha.-hydroxy-4-nitro-.alpha.-(4-nitrophenyl)-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.

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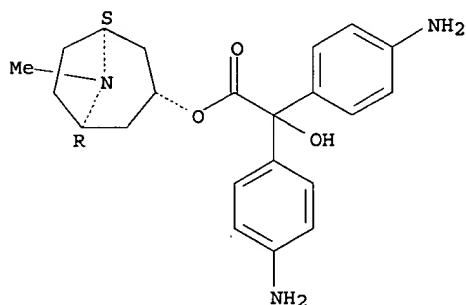
102

31, 32

RN 172883-94-2 CAPLUS

CN Benzeneacetic acid, 4-amino-.alpha.-(4-aminophenyl)-.alpha.-hydroxy-,
8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, exo- (9CI) (CA INDEX NAME)

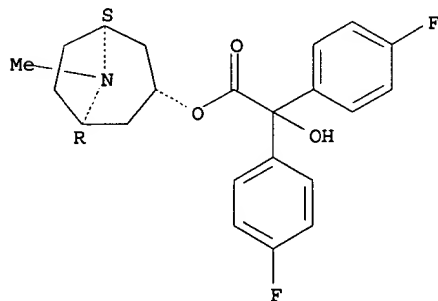
Relative stereochemistry.



RN 172883-95-3 CAPLUS

CN Benzeneacetic acid, 4-fluoro-.alpha.-(4-fluorophenyl)-.alpha.-hydroxy-,
8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



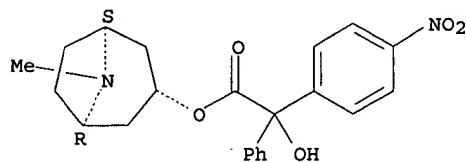
102

31, 35

RN 172883-98-6 CAPLUS

CN Benzeneacetic acid, .alpha.-hydroxy-4-nitro-.alpha.-phenyl-,
8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



102

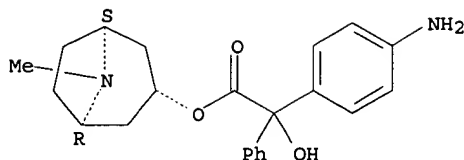
31, 32

RN 172883-99-7 CAPLUS

CN Benzeneacetic acid, 4-amino-.alpha.-hydroxy-.alpha.-phenyl-,
8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, exo- (9CI) (CA INDEX NAME)

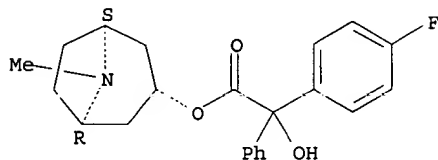
Relative stereochemistry.

09965766



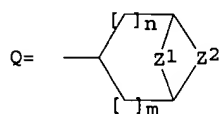
RN 172884-00-3 CAPLUS
 CN Benzeneacetic acid, 4-fluoro-.alpha.-hydroxy-.alpha.-phenyl-,
 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L17 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS
 AN 1993:428006 CAPLUS
 DN 119:28006
 TI Preparation of tropanyl methobromide esters and analogs as
 anticholinergics
 IN Banholzer, Rolf; Bauer, Rudolf; Reichl, Richard
 PA Boehringer Ingelheim KG, Germany
 SO Ger. Offen., 21 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4108393	A1	19920917	DE 1991-4108393	19910315
	CA 2105575	AA	19920916	CA 1992-2105575	19920305
	WO 9216528	A1	19921001	WO 1992-EP489	19920305
	W: AU, CA, CS, FI, HU, JP, KR, NO, PL, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
	AU 9213457	A1	19921021	AU 1992-13457	19920305
	AU 662128	B2	19950824		
	EP 579615	A1	19940126	EP 1992-905643	19920305
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
	HU 65132	A2	19940428	HU 1993-2611	19920305
PRAI	JP 06505718	T2	19940630	JP 1992-505496	19920305
	CZ 281509	B6	19961016	CZ 1993-1917	19920305
	PL 179673	B1	20001031	PL 1992-300630	19920305
	SK 281511	B6	20010409	SK 1993-949	19920305
	AT 202778	E	20010715	AT 1992-905643	19920305
	ES 2160577	T3	20011116	ES 1992-905643	19920305
	ZA 9201875	A	19930913	ZA 1992-1875	19920313
	IL 101225	A1	19960514	IL 1992-101225	19920313
	NO 9303274	A	19931112	NO 1993-3274	19930914
	US 5654314	A	19970805	US 1995-412407	19950328
OS	US 5770738	A	19980623	US 1995-412408	19950328
	DE 1991-4108393	A	19910315		
	WO 1992-EP489	A	19920305		
GI	US 1993-117199	B1	19931202		
	MARPAT 119:28006				



AB ZC02A [A = bicyclic group Q; Z = CR1R2R3; R1 = H, OH, CH2OH, alkyl,
 alkoxy; R2, R3 = Ph, thienyl, furyl, pyridyl, (cyclo)alkyl, etc.; CR2R3 =
 annelated cycloalkyl or heterocyclyl; Z1 = CH2, NR, etc.; R = (halo)alkyl,

hydroxyalkyl; Z2 = (CH₂)₂₋₃, CH:CH, 2,3-oxiranediy, etc.; m = 0-2; n = 1, 2; m + n = 1 to req. 3] were prepd. as anticholinergics (no data). Thus, ClCPh₂COCl was condensed with scopine and the product condensed with MeBr to give benzilic acid scopine ester methobromide.

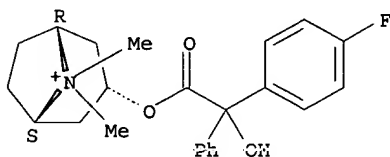
IT 145616-96-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as anticholinergic)

RN 145616-96-2 CAPLUS

CN 8-Azoniabicyclo[3.2.1]octane, 3-[[[(4-fluorophenyl)hydroxyphenylacetyl]oxy]-8,8-dimethyl-, bromide, endo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● Br⁻

L17 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2002 ACS

AN 1967:473724 CAPLUS

DN 67:73724

TI Esters of tropine, 1-(diethylamino)-2-propanol, and .beta.-(diethylamino)ethanol

AU Zakharova, N. A.; Khromov-Borisov, N. V.; Indenbom, M. L.

SO Zh. Org. Khim. (1967), 3(6), 1128-36

CODEN: ZORKAE

DT Journal

LA Russian

GI For diagram(s), see printed CA Issue.

AB A series of tropine (I), MeCH(OH)CH₂NEt₂ (II), and CH₂(OH)CH₂NEt₂ (III) esters with Ph₂C(OH)CO₂H (IV), Ph(p-MeOC₆H₄)C(OH)CO₂H (V), (p-MeOC₆H₄)₂C(OH)CO₂H (VI), PhCClCO₂H (VII), 2,2'-biphenyleneglycolic acid (VIII), 2,2'-biphenyleneacetic acid (IX), Ph(p-MeOC₆H₄)-CHCO₂H (X), and (p-MeOC₆H₄)₂CHCO₂H (XI) was prepd. The compds. were of potential interest as anticonvulsants, in treatment of parkinsonism, and as central/cholinolytic agents. The esters were prepd. by transesterification of (for example) IV Et ester with I.HCl salt; IV Et ester was prepd. from its Ag salt and EtI. Thus, 0.1 mole IV soln. in 150 ml. abs. alc. was combined with 0.1 mole KOH and the mixt. evapd. to dryness. The residue was dissolved in water, charcoaled, and boiled with 0.1 mole AgNO₃. IV Ag salt pptd. in 85-97% yield. To a mixt. of 0.05 mole IV Ag salt a soln. of 0.05 mole EtI in 72 ml. anhyd. benzene was added. The mixt. was heated approx. 30 min., filtered, and distd. to give 72.2% yield of IV Et ester, b₃₋₅ 150-75.degree.. Similarly other Et esters were prepd. (acid, ester % yield, b.p./mm. or m.p. given): V, 77.4, 197-202.degree./5; VI, 81.5, 215-20.degree./3-5 (m. 92-8.degree.); VIII, 69.0, m. 87-90.degree.. A mixt. of 0.04 g. I, 0.08 g. Na, and 0.02 mole VI Et ester was kept at 130-40.degree. 4-5 hrs. in vacuo increasing from 30-40 mm. to 8-12 mm. The melt was stirred with 120-150 ml. HCl soln. The org. layer was sepd. [1.8 g. of an insol. ppt. was filtered to give (p-MeOC₆H₄)₂CO m. 143-4.degree. (alc.)]. The aq. layer was boiled with charcoal, filtered, and neutralized with 2N NH₄OH soln. in the cold. The ppt. was filtered off, redissolved in abs. alc., and acidified with alc. HCl soln. to give 49.4% ester [m. 200-2.degree. (abs. alc.)] of VI and tropinium chloride. Similarly, other esters of tropinium salt were prepd. (acid and % yield and m.p. of ester given): IV, 28.0, 238.degree. (abs. alc.); V, 48.2, 194-5.degree. (Et₂O-alc.); VIII (VIIIa), 48.9, 240-1.degree. (Et₂O-alc.). The ester [m. 207-10.degree. (Me₂CO)], of IX and tropinium chloride, was prepd. by a direct reaction between I and tech. IX chloride, m. 65-73.degree., in 74.4% yield. A mixt. of 9 g. ester of IV and tropinium-chloride and 16.5 ml. SOCl₂ was boiled 4 hrs. Removal of excess SOCl₂, extn. with acetone, and crystn. of the residue gave 62% ester [m. 126-8.degree. (benzene-ligroine)] of VII and tropinium chloride. A mixt. of 0.04 mole V, 30 g. SnCl₂, 80 ml. AcOH, and 60 ml. HCl was stirred 2 hrs. at 30-5.degree. to give 68.5% X. Similarly, XI was prepd. in 61% yield. The acids were converted to the chlorides with SOCl₂ in 84% (X chloride) and 80% (XI chloride) yields. Esterification of 0.05 mole II with equiv. of X by heating 2 hrs. 115-25.degree. in 15 ml. PhMe gave 53.6% ester of X and II m. 133-5.degree. (Et₂O-alc.). In the same way the

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ester of XI and II, m. 112-14.degree. (Et2O-alc.), and ester of IX and II, m. 165-6.degree. (acetone) were prepd. in 30.8 and 77.1% yields, resp. Condensation of Cl(CH2)2NEt2 with IX, X, or XI by boiling in PhMe gave the corresponding ester of IX and III m. 143-4.degree. (PhMe) (65.5%); ester of X and III m. 128-30.degree. (benzene-ligroine) (57.4%), and ester of XI and III m. 155-6.degree. (benzene-ligroine) (60.5%).

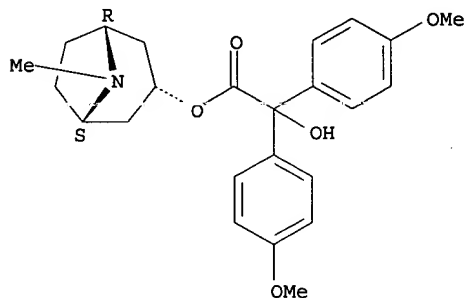
IT 16658-58-5P 16658-60-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 16658-58-5 CAPLUS

CN 1.alpha.H,5.alpha.H-Tropan-3.alpha.-ol, 4,4'-dimethoxybenzilate (ester), hydrochloride (8CI) (CA INDEX NAME)

Relative stereochemistry.

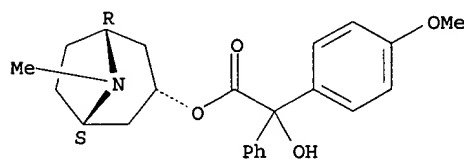


● HCl

RN 16658-60-9 CAPLUS

CN 1.alpha.H,5.alpha.H-Tropan-3.alpha.-ol, 4-methoxybenzilate (ester), hydrochloride (8CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl